

PREDICTING *para-ortho* CONVERSION IN AMMONIA

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We present a combined theoretical and experimental study of the hyperfine-resolved spectrum of ammonia and its deuterated isotopologues. The calculations have been performed using the variational approach TROVE, a new spectroscopically determined potential energy surface, and *ab initio* quadrupole, spin-spin, and spin-rotation coupling surfaces. The computed spectroscopic line lists cover transitions between levels with rotational excitations $J = 0 \dots 20$ and vibrational band centers with up to 8000 cm^{-1} above the zero-point-energy level.

For the spectroscopic observation of the *para-ortho* interconversion we use mid-infrared frequency comb spectroscopy in both ammonia vapour and a cold molecular beam. Furthermore, its modulation by external electric field is discussed. Our theoretical model, i.e., the underlying potential energy surface will be refined using the experimentally observed transitions.